Initiative for Simulation and Modeling for Global Security, Prosperity, and Sustainability

Town Hall Meeting

Lawrence Berkeley National Lab

April 17, 2007

Group 3: Enhance understanding of the roles & functions carried out by microbial life on Earth

Moderators: Victor M Markowitz and Nikos C. Kyrpides

Outlook for Next 5-10 Years

❖ Goals

- Sequence data for a large number (3,000 to 10,000) of representative organisms of culturable microbial species as well as hundreds of microbial communities
- Functional genomics (microarray, proteomics, etc.) data for hundreds of cultured microbes and several microbial communities
- New bio-engineering targets for production of bio-fuels, such as cellulose-degrading organisms, ethanol producers, etc.
  - Will entail large scale data processing & functional characterization, for genomes and metagenomes

❖ Rationale

There is clear need for powerful computing infrastructure to support all aspects of microbial genome and metagenome data processing and functional characterization

☞ See Kyrpides-Ivanova, Edwards, and Sjolander presentations

Challenges

❖ Data quality & semantics
- Accuracy, consistency, completeness of annotations
- Compatibility with metabolic modeling and simulation requirements

❖ Data analysis
- Development of new, more efficient methods
- Visualization for effective exploration of large data sets

❖ Data integration
  Data generated using different technologies and/or of different (e.g. sequence, microarray, proteomic) types

❖ Infrastructure
- Computing
- Data management

Current Status

❖ Computing infrastructure
  Systems such as IMG are caught between the promise of powerful (super) computing centers at national labs and the reality of
  - very limited (sometimes no) access to these resources
  - resources lacking the necessary environment for running large scale applications such as blast searches and HMMs
  ☞ See Oehmen and Konerding presentations

❖ Data management
  Lack of coordination between microbial genome resources, such as LBNL's MicrobesOnline, JGI's IMG, and ANL's SEED and PUMA cause
  - Repeated computations to determine (e.g., homologous) gene relationships
  - Difficulty assessing consistency of functional characterization across systems
  ☞ Problem complexity will increase with scale up of sequencing and functional genomics experiments

What is Needed

❖ Foundation

New frontiers in computing, data management, and data analysis aimed at serving microbial genome and metagenome applications require <u>retrofitting</u> existing foundation, including
- Revising & coordinating (e.g., federating) existing systems/processes
- Establishing metrics for data/system/infrastructure quality

❖ Organization

Setting goals and advancing microbial genome and metagenome studies require close <u>partnerships</u> between computer scientists and biologists, that would involve
- Setting clear milestones and goals for computer science in order to determine practical (as opposed to theoretical) effect on biology studies
- Joint management of large computing and data management projects

Major risks

❖ False start

Setting new frontiers without a clear and detailed review and understanding of current problems and shortcomings

❖ Credibility gap

Gap between the promise and reality of computing and data management support for microbial genome studies needs to be addressed, including

Eliminate the disconnect between computer science R&D and bio research studies
- Bio studies need "production" data management & computing infrastructure
- Computer science R&D tends to produce illustrative "prototype" systems and applications that have little or no practical value for real-life biological studies